Triethanolamine
102-71-6 | DTXSID9021392

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.72 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.04e-01

Confidence level: 7.83e-01

Nearest Neighbors from the Training Set

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Triethanolamine
Measured: 6.70
Predicted: 6.72

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N-Methyldiethanolamine
Measured: 8.39
Predicted: 8.36

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N-Nitrosodiethanolamine
Measured: 7.45
Predicted: 6.23

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Ethyl diethanolamine
Measured: 7.51
Predicted: 7.70

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Triisopropanolamine
Measured: 4.34
Predicted: 3.33